

Bond rearrangement in NH_3 under slow highly charged ion impact

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Synopsis Ultra fast bond rearrangement in ammonia is observed under slow highly charged ion impact.

The migration of protons is an important process from the point of view of isomerization of molecules during chemical reactions. A number of reports are available in the literature on the formation of H_2^+ and H_3^+ ions as these are an essential facet in the reactions through which many molecules, like, H_2O , CH_4 , NH_3 and several other hydrocarbons are thought to be formed in the astrophysical environment. Recently the rearrangement of H-atoms in NH_3 has been reported by few workers [1, 2]

In the present experiment [3], the low energy highly charged Argon ions are generated from an electron cyclotron resonance source and are made to collide with a gas jet of NH_3 under single collision condition. The recoil ions and ejected electrons are extracted in opposite directions by applying a homogeneous electric field; these are detected by a micro channel plate and a channel electron multiplier, respectively. The position information of the recoil ions is obtained by a delay line anode. The momentum of an ion is obtained by measuring its time of flight from collision center to the detector and its position simultaneously. Triple ion coincidence technique is employed to study the dynamical properties of the precursor ion NH_3^{q+} ($q=3-5$) giving rise to three fragment ions. Only the fragmentation channels involving rearrangement of hydrogen atoms are discussed here.

We have observed that the dissociation of NH_3^{q+} ($q=3-5$) occurs concertedly where the H^+ , H_2^+ and N^{p+} ($p=1-3$) ions fly out of plane. Further, the bond rearrangement, though having a low cross section, is faster in comparison to the Coulomb explosion. The rearrangement process is observed in case of multiply charged NH_3 also which is contrary to earlier reports where rearrangement is suggested to occur for up to doubly charged parent ions only. The kinetic energy release value for the dissociation of NH_3^{2+} is found to be consistent with the earlier theoretical calculations

and the measurements.

To understand the structure of dissociating NH_3^{2+} , the *ab initio* calculations at the unrestricted Hartree Fock level under adiabatic approximation are performed (see, Figure 1). An interesting result is observed that the dissociation channels involving rearrangement of H-atoms originate from the doubly charged NH_3 only when it has a planar structure. However, the neutral NH_3 has a trigonal pyramidal geometry in its ground state.

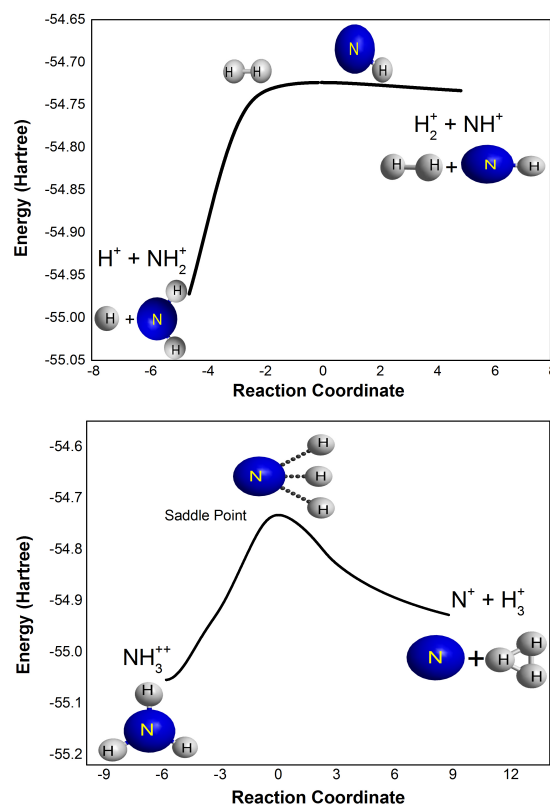


Figure 1. Reaction Path for the dissociation of NH_3^{2+} into bond rearrangement channels considering its initial geometry to be planar.

References

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